Isoamyl ether 544-01-4 | DTXSID8052198

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 203 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.73e-01

Confidence level: 6.83e-01

Nearest Neighbors from the Training Set

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1-Nonanol

Measured: 77.6 Predicted: 101

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1-Decanol

Measured: 389 Predicted: 347 Image not found

Ethyl heptanoate **Measured:** 407

Predicted: 284

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1-Octanol

Measured: 36.3 Predicted: 42.5 Image not found

Ethyl octanoate
Measured: 1050
Predicted: 617